Understanding the Wetting Behavior of Fluids at Heterogeneous Surfaces

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We first describe our recent efforts aimed at development of Monte Carlo simulation methods for determining the wetting properties of fluids at solid surfaces. Our strategy involves calculation of the surface excess free energy (also referred to as the interface potential) as a function of the surface density of a fluid in contact with the substrate at a specified temperature and chemical potential. The shape of this curve provides qualitative insight regarding the system's wetting behavior (e.g. partial wetting, complete wetting) and quantitative analysis provides macroscopic interfacial properties, such as the spreading coefficient and interfacial tension. We describe how components of the interface potential are obtained via grand canonical transition matrix Monte Carlo simulation and various expanded ensemble Monte Carlo simulation strategies. We then show examples of the application of this general strategy to heterogeneous surfaces. Specifically, we examine the effect of nanoscale geometric surface roughness (substrates with hills and valleys that have heights and widths in the 1-25 nm range) on wetting behavior. We work with two model fluids: Lennard-Jonesium and SPCE water. We focus on the evolution of the contact angle with variation of the amplitude and length scale of geometric heterogeneities. Our simulation-based results are compared with macroscopically-based expressions for describing the influence of roughness, such as those due to Wenzel and Cassie.